COMPUTER SIMULATION STUDY OF PHYSICAL PROPERTIES OF NANOSIZED BIOSTRUCTURES

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Abstract. Computer simulation study of bionanoparticles' physical properties, method of estimation of electromagnetic (EM) spectrum and resonance wave-length ranges is considered. Solution of well-established classical electrodynamics boundary problem is applied to nanobioparticles characterization. Possibility of appreciation EM spectrum and EM field distribution is demonstrated for virion of Tobacco Mosaic Virus (TMV), which is modeled by the particle of cylindrical shape and definite geometrical, electrical and magnetic characteristics. A set of resonance wavelength is observed in ultraviolet (NUV-EUV) range of TMV particle's spectrum.

1. Introduction

Study of biostructure's physical characteristics, scattering and absorbtion properties, estimation of electromagnetic (EM) spectrum and resonance wave length ranges is important for characterization of nano-micro-scaled particles and determination of biostructures unique spectral signatures, so essential in bio-agents detecting and identification systems. Investigation of EM field distribution makes possible to have insight vision of the nanoparticles. Behavior of nano-micro sized pathogenic microorganisms such as bacteria, virus, organic and non-organic agents is selectively sensitive toward the electromagnetic (EM) field excitation. Elaboration of physical models of bioparticles, as well as computer simulation study of near and far EM field distribution in the areas of particles and surrounded medium is a possible way for investigation of physical properties of bio-particles of different morphology.

2. Method and approach

Method of estimation of spectral response on EM field & particle interaction is based on solutions of electrodynamics two (2D) or three (3D) dimensional boundary tasks [1, 2]. Obtained analytical expressions of EM fields are derived from rigorous solutions of Maxwell's and Helmholtz's equations and defined through the dimensionless parameters, diameters (d) over excitation wave-length (λ). It makes possible to apply the classical well-known approach to sub-micro particles characterization. Proposed method is used for investigation of viral particle's physical properties. EM near and far fields distribution, EM spectrum are proposed for viruses, having rod-like, prolate un-enveloped virions (e.g. Tobacco Mosaic Virus (TMV), bacteriophage M13). Virions, the extracellular infective forms of viruses are modelled by the particles of cylindrical shape of different structures, such as homogeneous dielectric particles and inhomogeneous through the radius, also particles of core-shell structure reflecting the properties of ribonucleic acids (DNA or RNA) of viruses and capsid's proteins. Shape, structure and the set of geometrical, magnetic and electrical characteristics are the main parameters defining the particles' EM spectral properties. Advantage of simulation study of complex molecular systems such as virions in contrast of measuring experiments associated with weak signals detection is noteworthy.

3. Results

Computer simulation (based on MatLabR2013b software) was carried out for TMV particles characterization. Parameters of TMV particle are obtained from scientific publications based on different measuring technics [3]. Length of TMV virion is 280-300 nm, outer and inner diameters of capsid are $d_2 = 18$ nm and $d_1 = 4$ nm, correspondingly. Dielectric permittivitys of core (RNA) - ε_1, shell (capsids proteins) - ε_2, surrounded medium - ε_3. Two models are used for simulation study of TMV virion: homogeneous and core-shell structured cylinders. Computer simulation shows that expected resonant spectral response is observable on far-field ($r >> 2d_2^2/\lambda$) characteristics (Fig.1), resonant vibrational frequencies of whole TMV particle may be associated to scattering cross section maximums.

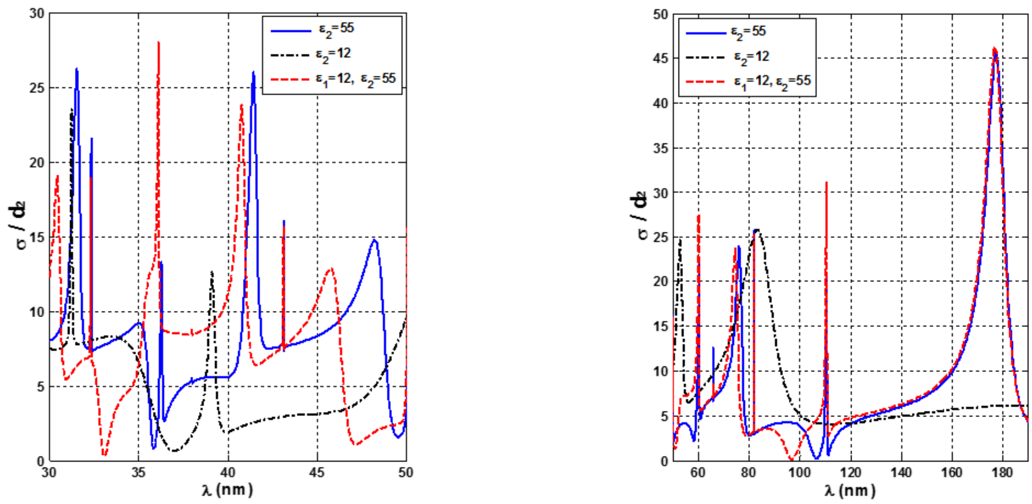
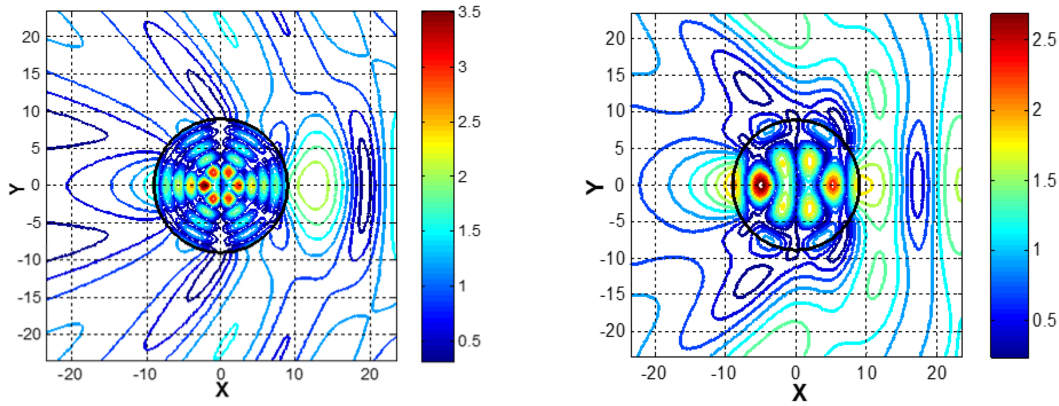


Fig.1. Forward scattering cross section (σ / d_2) vs excitation wave length (λ).
Cylindrical model: diameter d_2 =18 nm, dielectric permittivity $\varepsilon_2 = 55$ (solid blue), 12 (dash-dot black), Core-shell model (dash red): diameters $d_2 = 18$ nm (outer) and $d_1 = 4$ nm (inner), dielectric permittivitys: $\varepsilon_1 = 12$ (core), $\varepsilon_2 = 55$ (shell); $\varepsilon_3 = 1$ (surrounding medium).

Near-field distribution presented in a form of isolines of EM field amplitudes (Fig.2), indicates the locations of energy maximums inside and outside of particle.



a) b)

Fig. 2 Isolines of EM field amplitudes for cylindrical model of TMV virion, in the range of (- λ ,+ λ).
Diameter of cylinder: d_2 =18 nm; dielectric permittivitys: of cylindrical particle - $\varepsilon_2 = 55$ (a), 12 (b), surrounding medium - $\varepsilon_3 = 1$, excitation wave length λ = 23.5 nm, (X,Y) plane is perpendicular to the axis of cylinder.

Conclusions

Method of estimation EM field characteristics and resonant wave ranges based on computer simulation is developed. Data analysis revealed the strong dependence of field characteristics on electromagnetic plus geometrical parameters and wave length in resonant wave range. Possibility of determination of resonant frequencies of virions is demonstrated. Simulated EM spectra as the specific signature of bio-particles of a given parameters is proposed for consideration.

References

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